Amendments to the Claims:

1. (Currently Amended). A method for calculating the similarity of at least one chemical compound to at least one chemical probe, comprising the steps of:

(a) utilizing at least one chemical descriptor for each of a plurality of compounds, each descriptor comprising a row of a molecule-descriptor matrix *X*;

(b) representing each compound as a column of the molecule-descriptor matrix, the entries of the molecule-descriptor matrix comprising a ~~mathematical function of the weighting~~ frequency of each descriptor for each compound;

(c) performing a partial singular value decomposition (SVD) of the molecule-descriptor matrix to produce resultant matrices;

(d) creating a chemical probe descriptor matrix for the at least one chemical probe, the entries of the chemical probe descriptor matrix comprising a ~~mathematical function of the weighting~~ frequency of each descriptor for each chemical probe;

(e) using at least one of the resultant matrices to calculate the similarity between the at least one chemical probe and at least one compound of the molecule descriptor matrix; and

(f) providing an output indicating the similarity between the at least one chemical probe and the at least one compound.

2. (Previously Presented). The method as recited in claim 1, wherein each of the at least one chemical descriptors comprise at least one of an atom pair descriptor and a topological torsion descriptor.

4. (Previously Presented). The method as recited in claim 1, wherein said performing step comprises the steps of:

generating resultant matrices P, Σ and Q^T, such that molecule-descriptor matrix $X = P\Sigma Q^T$, wherein

P is a mxr matrix, called the left singular matrix (r is the rank of X), and its columns are the eigenvectors of XX^T corresponding to nonzero eigenvalues;

Q is a nxr matrix, called the right singular matrix, whose columns are the eigenvectors of X^TX corresponding to nonzero eigenvalues; and

Σ is a rxr diagonal matrix whose nonzero elements, σ_1, σ_2, ..., σ_r called singular values, are the square roots of the eigenvalues and have the property that $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r$.

5. (Previously Presented). The method as recited to claim 4, wherein said similarity between the at least one chemical probe and at least one compound of the molecule descriptor matrix is computed in accordance with the following steps:

generating a reduced dimension approximation of X of rank k, defined as $X_k = P_k\Sigma_k Q^T_k$, k < r;

generating a pseudo-object, denoted as O_F, where $O_F = F^T P_k \Sigma^{-1}_k$, and where F is a molecule-descriptor vector for the at least one chemical probe; and

taking a dot product of O_F with one or more columns of Q^T_k respectively corresponding to the at least one compound.

6. (Previously Presented). The method as recited in claim 5, wherein σ_{k+1} to σ_r are equal to zero for Σ_k.

7. (Previously Presented). The method as recited in claim 5, wherein σ_l to σ_k are equal to one for Σ_k.

8. (Currently Amended). The method as recited in claim 7, wherein Σ_k ~~comprises an~~ is the identity matrix I.

22. – 29. (Canceled).